

## IV.B.4j Safety Analysis and Applied Research on the Use of Borane-Amines for Hydrogen Storage

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### Accomplishments

- Completed literature searching
- Collected Material Safety Data Sheets
- Collected additional reactivity, stability and toxicity information
- Collected anecdotal observations
- Completed and disseminated survey document
- Completed and distributed an electronic database via CDs

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### Introduction

This project has completed a thorough technical survey of all knowledge relating to amine-borane compounds and borazines. Insights gained from this survey are being applied across the Chemical Hydrogen Storage Center of Excellence to ensure that the design and synthesis of amine-borane based hydrogen storage materials meet or exceed all applicable safety and toxicity standards as defined by DOE.

This project will conduct applied research studies of ammonia-borane and N-substituted amine-borane compounds. Insights gained from these studies will be applied toward the design and synthesis of hydrogen storage materials that will meet the DOE 2010 hydrogen storage targets, especially gravimetric and volumetric capacity.

### Approach

We will complete a survey of technical articles, patents and anecdotal information that deal with the preparation, physical properties, chemical properties and safety aspects of amine-borane compounds and borazines. Chemical Abstracts on-line will be the main tool used to search the literature. Anecdotal observations will be collected by telephone, e-mail and/or personal visits to organizations and research groups currently or formally active in borane-amine chemistry. A report on hazards associated with preparation and handling of borane-amines, and means to mitigate these hazards, will be disseminated to all partners in the Chemical Hydrogen Storage Center of Excellence.

We will prepare various N-substituted amine-borane compounds and determine their solubility and stability in a few inert high-boiling solvents. The best

### Objectives

- Provide guidance for safe handling of amine-borane compounds throughout the Chemical Hydrogen Storage Center of Excellence
- Evaluate hydrogen on-board generation and off-board regeneration capability and capacity of N-substituted amine-borane compounds to determine if a laboratory scale system can be developed that safely meets the DOE 2010 target of 6 wt% hydrogen

### Technical Barriers

This project addresses the following technical barriers from the Storage section (3.3.4.2) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- (B) Weight and Volume
- (C) Efficiency
- (R) Regeneration Processes

### Technical Targets

- Safety Analysis
- DOE 2010 target of 6 wt% hydrogen

candidates will be studied to see if a safe decomposition can be achieved at a reasonable temperature and if an expected borazine product is produced. This will be done by studying the effect of time and temperature on the evolution of hydrogen from these solutions and by isolation and identification of any intermediates. In collaboration with other Center partners, catalytic processes will be studied for the evolution of hydrogen from these solutions to see if a system can be developed that cleanly forms a non-volatile product plus pure hydrogen at a temperature low enough to use the waste heat from fuel cells.

## Results

A complete literature search for the preparation, physical properties, chemical properties and safety aspects of amine-borane compounds and borazines was completed. Material Safety Data Sheets were collected from all manufacturers of amine-borane compounds and borazine. Additional reactivity, stability and toxicity information was collected from various manufacturers of amine-borane compounds and borazine. Anecdotal observations were collected from organizations and research groups (outside of the Chemical Hydrogen Storage Center of Excellence) that are currently or were formerly active in amine-borane chemistry.

The above information was condensed in a survey document report which detailed safety aspects, synthesis, properties and applications of N-B-H compounds and materials. An electronic copy of this report was disseminated to all partners in the DOE Chemical Hydrogen Storage Center of Excellence. In addition,

an electronic database with links to copies of essentially all 440+ references was placed on a CD and copies were distributed to each interested partner in the DOE Chemical Hydrogen Storage Center of Excellence.

## Conclusions and Future Directions

All currently available information on the safety, toxicity, stability and reactivity of amine-borane compounds seems to indicate that these materials are viable candidates for chemical hydrogen storage.

Laboratory efforts are now being directed toward the development of an improved process for the preparation of ammonia-borane. This work will result in the isolation of laboratory quantities of ammonia-borane that will be provided to interested partners in the Chemical Hydrogen Storage Center. In addition, we will prepare various N-substituted amine-borane compounds and determine their solubility and stability in a few inert high-boiling solvents. The best candidates will be supplied to other Center partners to see if safe decomposition can be achieved at a reasonable temperature and if a non-volatile N-B-H product is produced.

## FY 2006 Publications/Presentations

1. Survey document entitled: "*Ammonia-Borane and Related N-B-H Compounds and Materials: Safety Aspects, Properties and Applications.*"
2. A poster summarizing the project status was presented at the DOE Annual Merit Review Meeting (May 2006).